Neél order in square and triangular lattice Heisenberg models

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Using examples of the square- and triangular-lattice Heisenberg models we demonstrate that the density matrix renormalization group method (DMRG) can be effectively used to study magnetic ordering in two-dimensional lattice spin models. We show that local quantities in DMRG calculations, such as the on-site magnetization M, should be extrapolated with the truncation error, not with its square root, as previously assumed. We also introduce convenient sequences of clusters, using cylindrical boundary conditions and pinning magnetic fields, which provide for rapidly converging finite-size scaling. This scaling behavior on our clusters is clarified using finite-size analysis of the effective σ-model and finite-size spin-wave theory. The resulting greatly improved extrapolations allow us to determine the thermodynamic limit of M for the square lattice with an error comparable to quantum Monte Carlo. For the triangular lattice, we verify the existence of three-sublattice magnetic order, and estimate the order parameter to be $M = 0.205(15)$.

Two-dimensional (2D) quantum lattice systems studied in condensed matter physics can be divided into two types: those with a sign problem in quantum Monte Carlo (QMC), and those without one. This is because recent developments in QMC[1, 2, 3] have enabled remarkably accurate large-scale studies of the latter systems, such as the square-lattice Heisenberg model (SLHM) [4]. In contrast, the former systems, such as the triangular lattice Heisenberg model (TLHM) and other models with geometric frustration, are often the subject of controversy even regarding questions of what type of order, if any, is present. For the TLHM, it is only recently that the rough agreement between several theoretical[5] and numerical[6, 7, 8] methods has made a convincing case that the model has three-sublattice, non-collinear $120°$ order.

The density matrix renormalization group[9] (DMRG) is not subject to the sign problem, it has an error which can be systematically decreased by keeping more states, and even with modest computational effort it is extremely accurate for one dimensional and ladder systems. For 2D systems, the computational effort grows exponentially with the width. Ameliorating this effect is the very systematic behavior of the DMRG results versus the number of states kept, enabling the use of extrapolations to improve the accuracy. The extrapolation of the energy versus the truncation error ε (also known as the discarded weight) to the limit $\varepsilon \to 0$ often can improve the accuracy of the energy by nearly an order of magnitude. For observables other than the energy, extrapolation has been more problematic and is much less used.

In this Letter we show that the difficulty in extrapolating local measurements A is due to the incorrect assumption that the error $\Delta A \sim \varepsilon^{1/2}$. In fact, the simplest way to measure local quantities within DMRG makes ΔA *analytic* in ε. The resulting improved extrapolations greatly improve one's ability to measure order parameters in two dimensional systems. We demonstrate this approach with a study of the SLHM and TLHM systems. For the SLHM, the results for the on-site magnetization, extrapolated in both truncation error and system size, are about as good as the best published QMC.[4, 10]

For the TLHM, our new results for the magnetization are comparable to the best series expansion[8] and GFMC[7] results.

Another limitation of DMRG is a large loss of accuracy if periodic boundary conditions (BCs) are used lengthwise. As part of our treatment, we demonstrate an approach using cylindrical BCs on $L_x \neq L_y$ clusters and pinning magnetic fields. We show that with an appropriate choice of the aspect ratio $\alpha = L_x/L_y$, quantities such as the staggered magnetization scale much more rapidly to the thermodynamic limit than in widely used methods based on correlation functions on $L_x = L_y$ clusters with periodic BCs in both directions.

We consider the $S = \frac{1}{2}$ Heisenberg model

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad (1)$$

on square and triangular lattices, where $\langle ij \rangle$ denotes nearest neighbor sites, and we set $J = 1$. We consider $L_x \times L_y$ systems with periodic BCs in the y direction, and open BCs with pinning in the x direction. For the SLHM we consider both the standard orientation of the lattice and one tilted by $45°$. In all cases we apply a staggered pinning field corresponding to infinite pinning on the edges of an auxiliary $(L_x + 2) \times L_y$ system, e.g. ± 0.5 for the standard orientation SLHM. Since our DMRG program conserves total S_z, for the TLHM it is not possible to pin all three sublattices simultaneously. Instead, we only pin in the z direction, pinning one sublattice (pointing down), with the other two free to rotate in a cone. Thus we expect one sublattice in large systems to exhibit $\langle S_z \rangle = -M$, and the other two $+M/2$.

We focus on the resulting onsite magnetization $M_C = |\langle S_z \rangle|$ in the center column of the system. For any fixed aspect ratio $\alpha = L_x/L_y$, M_C approaches its thermodynamic limit, M_0, as $L_x, L_y \to \infty$. For $L_x \gg L_y$, the system looks more one-dimensional and we expect M_C to approach M_0 from below. For $L_y \gg L_x$, the strong pinning dominates and we expect an approach from above. We utilize intermediate values of α to accelerate the convergence with system size.
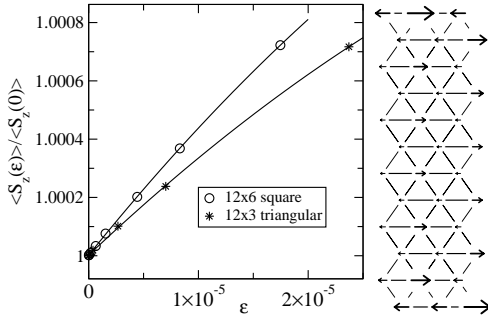
First we discuss the convergence of DMRG and extrapo-

FIG. 1: Measurements of $\langle S_z \rangle$ for a site in the middle of the cluster with pinning fields applied on the ends, as a function of the truncation error ε. The results are normalized by the result extrapolated to $\varepsilon \to 0$. The solid lines are quadratic fits to the data. The $6\sqrt{3} \times 3$ triangular cluster, rotated $90°$, is shown. The length of the arrows is proportional to $\langle S_z \rangle$, and pinning fields were -0.25, -0.25, 0.5.

lations in the truncation error ε—the sum of the density matrix eigenvalues which are discarded at each step. If the truncation of density matrix states were made starting from the exact ground state ψ_0, then the truncation error and energy error would vary as (to leading order) $\varepsilon \sim \Delta E \sim |\Delta \psi|^2$, where $\Delta \psi = \psi - \psi_0$, and ψ is the new approximate ground state[11]. For further discussion of energy extrapolation, see Refs. [9, 12, 13]. For measurements of an operator $\hat{A}$ other than the Hamiltonian, standard variational arguments imply an error proportional to $\langle \Delta \psi | \hat{A} | \psi_0 \rangle$, and thus $\propto \varepsilon^{1/2}$.

Consider the special situation where ψ is the lowest energy state within an incomplete basis B. Let C be the complement of B. Note that ψ is an exact eigenstate in the complete basis of a modified Hamiltonian in which the off-diagonal terms connecting B and C are set to zero. Label these coupling terms λV, where λ is an expansion parameter. Assuming ψ is close to the true ground state, ψ_0, $\lambda V \psi$ is small, and one can consider λV as a small perturbation. The leading term in $\Delta \psi$, neglecting energy denominators, is $\propto \lambda V \psi$, which is in C.

Now consider a change of basis for C, negating each basis function. This sends $\lambda \to -\lambda$. Since the energy is independent of the change of basis, $E(\lambda)$ is even and we expect analytic behavior for $E(\lambda^2)$. For the exact ground state ψ_0, the change of basis switches the sign of the C coefficients. The truncation error ε is (ideally[11]) the sum of the squares of these coefficients, and is therefore also an even function of λ. Consider an operator $\hat{A}$ which is block diagonal within the B/C split. Its expectation value would also be independent of the change of basis, and thus an analytic function of λ^2.

Within DMRG, the seemingly restrictive assumption that the operator $\hat{A}$ is block diagonal is easily satisfied for a local operator, such as S_z. Consider one particular DMRG step, and consider measuring an $\hat{A}$ which acts only on one or both of the central two sites, not part of the truncated left and right blocks. As part of the DMRG step, one finds the ground state ψ within the current reduced basis (B). Applying $\hat{A}$ on ψ creates a state which is exactly represented within this basis; therefore $\hat{A}$ is block diagonal. At this step only a few operators can be

measured accurately, but as the algorithm sweeps through the lattice all local operators can be measured.

To utilize this analytic behavior in an extrapolation, one assumes that successive sweeps, which become increasingly accurate as the number of states kept is increased, corresponds to decreasing λ. A better (but still approximate) description of the calculation is that the ground state is approached by taking the most significant states out of the truncated basis C and putting them in B, not by making λ smaller. We expect that in the limits of large numbers of states kept the two types of approaches are roughly equivalent. Then, both the energy and central-site operators should have polynomial (i.e. analytic) dependence on the truncation error, and one can expect well-behaved polynomial extrapolations.[14]

In Fig. 1, we show the behavior of $\langle S_z \rangle$ as a function of ε for two modest sized systems where essentially exact results could be obtained. The results show no signs of nonanalytic behavior as $\varepsilon \to 0$, and are fit nicely with a quadratic form. We have experimented to find a reliable way to extrapolate to $\varepsilon \to 0$, and have adopted the following simple procedure: we utilize only the most accurate decade of data available, and fit it with a cubic polynomial. The error bars assumed for the purpose of the fit are proportional to ε. The extrapolation can be checked by a fourth order fit, or a quadratic fit over a smaller range. If these extrapolations agree well, we take as a rough error estimate the empirical parameter 0.2 times the size of the extrapolation from the last data point. If the extrapolations do not agree well, we run the calculation longer if feasible, or raise the error estimate substantially.

The implications of the analytic behavior in ε are significant: local measurements for fixed ε are more accurate than previously thought, and the extrapolation $\varepsilon \to 0$ improves results substantially and provides reasonable error estimates.

We now turn to finite size effects. Previous QMC studies of the magnetization M have utilized correlation functions measured in periodic $L \times L$ systems, and extrapolation in $1/L$ for the quantity M_0^2. The leading term varies as $1/L$ with a substantial coefficient. The expansion in $1/L$ for the periodic $L \times L$ SLHM is known in detail from chiral perturbation theory, allowing Sandvik to determine $M_0 = 0.3070(3)$ using only systems up to $L = 16$[4]. For the TLHM, chiral perturbation results are not available, and less robust QMC methods must be used, making extrapolation to $L \to \infty$ much more difficult. For example, Capriotti et. al. extrapolated Green's function Monte Carlo results with $M^2 \geq 0.13$ for $L \leq 10$ down to $M_0^2 \sim 0.04$ for $L \to \infty$ to obtain $M_0 = 0.205(10)$. Other estimates[5] range as high as $M_0 = 0.266$.

It is known that the leading $1/L$-scaling of the order parameter M in the 2D Heisenberg systems is universal and is determined by the long-wavelength spectrum of the problem, namely by the massless spin waves.[15] We have analyzed the effect of the aspect ratio $\alpha = L_x/L_y$ on the scaling for pinned cylindrical and for periodic clusters using both finite-size scaling within an effective σ-model and the finite-size spin-wave theory (FSSWT). A key conclusion from both methods is that the coefficient in the $1/L$ correction to M de-
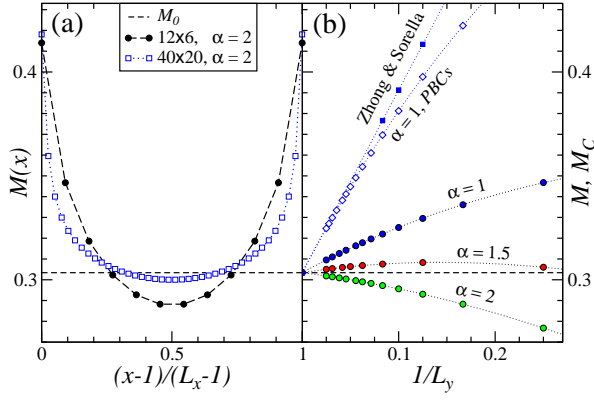
FIG. 2: (Color online). (a) FSSWT results for the SLHM showing the magnetization pattern $M(x)$ as a function of position along the cluster x, for two representative clusters. $M_0 = 0.3034$ is the bulk value of the staggered magnetization within the SWT. (b) M_C (M) vs $1/L_y$ results for various aspect ratios $\alpha = L_x/L_y$ by FSSWT for periodic BCs (upper two sets) and cylindrical BCs (lower two sets). In Ref. 16 M was extracted from the correlation function and differs from our results in the higher order ($1/L^2$) terms.

FIG. 3: (Color online). (a) $M(x)$ vs x DMRG results for the SLHM, for different aspect ratios. The line labeled "2D" and the solid diamond are the QMC $L \to \infty$ extrapolated result, $M_0 = 0.3070(3)$[4]. (b) M_C vs $1/L_y$ results from DMRG for the SLHM. The upper two curves are periodic QMC $\alpha = 1$ results for M[4] .

pends on α and, for special aspect ratios α_c, vanishes, leaving corrections of order $O(1/L^2)$. The two methods agree exactly on the values of α_c for nontilted and tilted square-lattice clusters: for periodic systems, $\alpha_c = 7.0555$, while for cylindrical systems, for M_C in the middle of the cluster, $\alpha_c = 1.7639$, almost exactly four times smaller. The values of α_c are controlled by the cluster geometry and boundary conditions through the placement of the allowed wavevectors near the zeros of spin-wave energy: for periodic SLHM systems, one has $\mathbf{k} = (\frac{2\pi i}{L_x}, \frac{2\pi j}{L_y})$, whereas for the cylindrical-pinned geometry case, $\mathbf{k} = (\frac{\pi i}{L_x+1}, \frac{2\pi j}{L_y})$. The factor of four improvement in the aspect ratio for the latter is due to the shift by $\frac{\pi}{L_x+1}$ away from the ordering vector. The effective-model analysis determines the $1/L$ correction term up to an unknown factor, but the zero crossing is independent of it.

The FSSWT produces parameter-free, approximate results for $M = |\langle S_z \rangle|$ for all sites. Fig. 2(a) shows $M(x)$ vs x for two representative clusters. Due to suppression of the long-wavelength spin fluctuations the magnetization is enhanced near the boundary. The asymptotic fall-off of the magnetization away from the edge can be shown to be $M(x) \approx M_0 + a/x$, where $a^{L=\infty} = (\pi\sqrt{8})^{-1}$. These FSSWT results are in a good agreement with the DMRG data for the SLHM in the non-tilted clusters shown in Fig. 3(a). One can see that already for the $L_x \times 6$ clusters M_C provides a good estimate of asymptotic 2D value M_0 when the aspect ratio is near $\alpha = 2$.

Figs. 2(b) and 3(b) show M_C versus $1/L_y$ for cylindrical BCs, obtained by the FSSWT and DMRG, respectively. Also shown are the results for the $L \times L$ systems with periodic BCs, in Fig. 2(b) by FSSWT from this work and from Ref. 16, and in Fig. 3(b) by QMC using standard correlation function methods, Ref. 4. Clearly, even for the same aspect ratio, the finite-size effects in the cylindrical BC clusters are 3-4 times
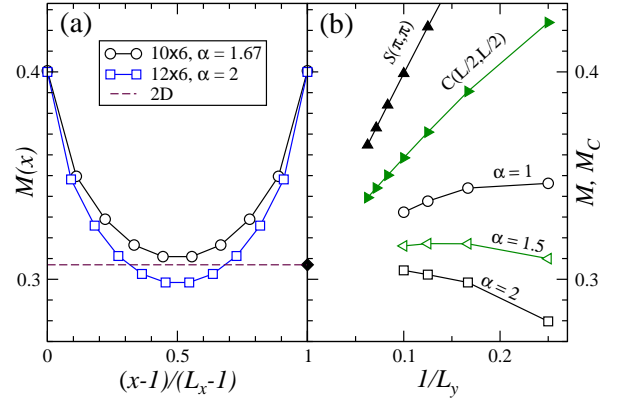
smaller than in the periodic systems. The FSSWT agrees precisely with the effective theory on the value of $\alpha_c = 1.7639$ for eliminating the leading $1/L$-term. This is in a good qualitative agreement with the DMRG data, but the DMRG seem to indicate consistently higher values of $\alpha_c \approx 1.9$. We have also performed QMC calculations[17] for the SLHM with periodic BCs. With the largest clusters up to 20×160 the "magic" aspect ratio is $\alpha_c \approx 7.5$, also higher than the effective theory value 7.0555. While we cannot exclude a change in the behavior on larger lattice sizes, this seems to indicate some insufficiency of the effective theory analysis.

In Fig. 3(b) DMRG results for M_C for lattices ranging up to 20×10 are shown. For the 20×10 system up to $m = 2400$ states were kept, with the run taking about 40 hours single-core time on a 2.6 GHz Mac Pro. This yielded a truncation error of order 10^{-6}, a variational energy with an estimated accuracy of a part in 10^4, an extrapolated energy accurate to a few parts in 10^5, and an uncertainty in M_C of about 0.0007.

More accurate DMRG results can be obtained for 45° tilted lattices[18], allowing more detailed fits. For example, on a $32/\sqrt{2} \times 8\sqrt{2}$ system, the energies and M_C were roughly 2 times more accurate than for the 20×10 nontilted system, and the finite size effects were smaller. The improved behavior comes from how DMRG sees the width of the system (the number of sites on the boundary of the left or right block) versus the physical dimension–the greater spacing by a factor of $\sqrt{2}$ in the tilted case accounts for the improvement. In Fig. 4(a) we show results for M_C versus $\alpha = L_x/L_y$ for various L_y near the value $\alpha = 1.925$ where the curves nearly intersect. The intersection of such curves as $L_y \to \infty$ provides a simple determination of both α_c and M_0. The resulting value of α_c, based on the available sizes, is somewhat larger than that given by FSSWT and the continuum analysis. The values of α are discrete because we have integral lattice dimensions. Performing a least squares fit of this data to the expression

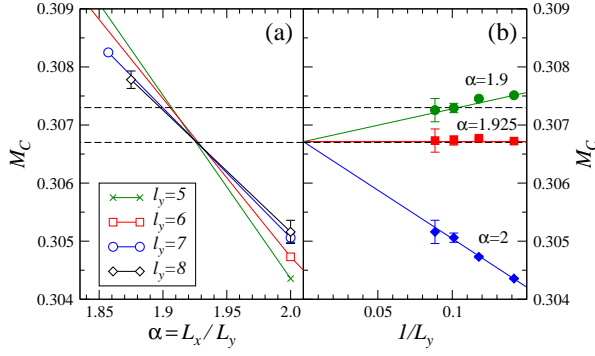$$M_C(\alpha, L_y) = M_0 + a(\alpha - \alpha_c)/L_y \qquad (2)$$

FIG. 4: (Color online). DMRG results for the $45°$ tilted SLHM. (a) The solid lines are straight segments connecting the discrete data points from different lattice sizes, with $L_y = l_y\sqrt{2}$. The two dashed lines show the bounds on the QMC result.[4] (b) A three parameter fit to the data from (a), as discussed in the text.

we obtain $M_0 = 0.3067$, $\alpha_c = 1.9252$, and $a = -0.1580$. In Fig. 4(b) we show a representation of this fit. The solid lines are based on the fit; the data points for $\alpha = 1.9$ and $\alpha = 1.925$ are obtained from linear extrapolation along the lines shown in (a). The result for M_0 is consistent with, and of comparable accuracy to the best QMC result.

For the triangular lattice, we have studied a variety of clusters and pinning fields; these results consistently supported that the triangular system has the three-sublattice $120°$ order found in other studies. The cluster orientation shown in Fig. 1 seems to be the most convenient and efficent for a DMRG analysis to obtain M_0. Our DMRG results for comparable lattice sizes are only slightly less accurate than for the SLHM.

Unfortunately, the finite size analysis for the TLHM is much less accurate. The allowed widths in the preferred geometry must be multiples of 3, and our results for $L_y = 12$ are of low accuracy, leaving only $L_y = 3, 6, 9$. Currently, we do not have comparable analytical guidance, such as predictions for the optimal aspect ratio, for the triangular case. In Fig. 5 we show results for the TLHM with this orientation and also for lattices rotated by $90°$. The scaling behavior appears to be quite similar to the SLHM, but with a somewhat
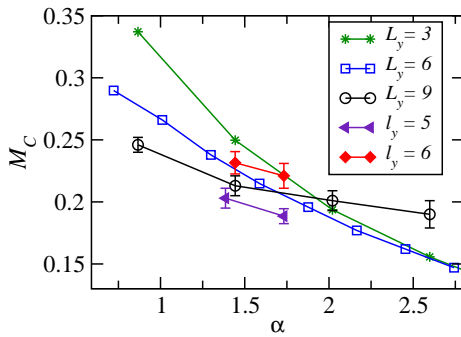
smaller $\alpha_c \sim 1.6 - 1.7$. Assuming this behavior, we estimate $M_0 = 0.205(15)$. The results for the tilted clusters seem to have larger finite size effects and are less useful. Our result is consistent with recent QMC and series expansions for M_0 for the TLHM[7, 8].

In conclusion, we have developed improved techniques for studying ordering in 2D lattice systems using DMRG, making DMRG competitive with QMC and series expansion methods for the 2D Heisenberg model on square and triangular lattices. These include proper scaling of local quantities with the discarded weight, and the use of non-traditional cluster geometries and BCs to improve finite-size scaling. These latter techniques can be used with other methods besides DMRG. We acknowledge the support of the NSF under grant DMR-0605444 (SRW), and the DOE under grant DE-FG02-04ER46174 (ALC).

FIG. 5: (Color online). M_C versus aspect ratio for various widths for the TLHM, from DMRG. The two curves labeled with l_y come from clusters rotated by $90°$, with $L_y = l_y\sqrt{3}$.

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